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MCNPX, VERSION 2.4.0

by

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1.0.   INTRODUCTION

The MCNPX 2.4.0 radiation transport code transports all particles at all energies. It is a superset of MCNP4C3 and MCNPX2.3.0 plus a number of new capabilities.

1.1.   Guarantee

MCNPX 2.4.0 is guaranteed. We are so confident of the quality of MCNPX 2.4.0 that we will pay $20 to the first person finding anything that does not meet or exceed the capabilities of MCNPX 2.3.0 and MCNP4C3. We also will pay a brand new $2 bill for any error in MCNPX 2.4.0 that has been inherited from its constituent codes.[1]

1.2.   Contents

1. Introduction
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2.0.   MCNPX 2.3.0 FEATURES NEW TO MCNP USERS

MCNPX 2.4.0 includes all of the features and capabilities of MCNPX 2.3.0 (based on MCNP4B), which was recently released to RSICC. MCNPX features that will be new to MCNP users include:

> Physics for 34 particle types;
> High-energy physics above the tabular data range;
> Photonuclear physics (already in MCNP4C2);
> Neutron, proton, and photonuclear 150-MeV libraries and utilization;
> Mesh tallies (tally fluxes, heating, sources, etc., in a superimposed mesh);
> Radiography tallies;
> Secondary-particle production biasing; and
> Autoconfiguration build system for compilation.

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1 Cash Award Fine Print: Offer subject to cancellation or modification without notice. A bug is defined as an error in the source code that we choose to correct. We make awards even for the most trivial or insignificant problems, but not for proposed code enhancements or proposed extended capabilities. Awards given only to the first MCNPX user reporting a problem. Reported problems must be reproducible, and awards are paid when the correction is integrated into a forthcoming MCNPX version. We believe MCNPX and its predecessor codes are the most error-free and robust Monte Carlo radiation transport capabilities. We challenge you to find a bug!

In particular, the mesh tallies enable users to plot source particle locations, fluxes, energy deposition, particle tracks, DXTRAN contributions, and other useful quantities on a superimposed tally grid. This capability is useful for all transport problems, not just high-energy problems.

3.0. MCNP4C3 FEATURES NEW TO MCNPX USERS

MCNPX 2.4.0 includes all the features and capabilities of MCNP4C3. Many of these features have not been in MCNPX before because, until now, MCNPX has been built on MCNP4B. Principal among these features not previously available in MCNPX are

> PC enhancements: MCNPX 2.4.0 is fully Linux and Windows capable;
> Easier geometry specification with macrobodies;
> Interactive geometry plotting;
> Improved variance reduction with the superimposed mesh weight window generator;
> Superimposed mesh plotting;
> Delayed neutrons;
> Unresolved resonance range probability tables;
> Perturbations for material-dependent tallies;
> ENDF/B-VI extensions;
> Electron physics enhancements (upgrade to ITS3.0);
> Weight window enhancements; and
> Distributed memory multiprocessing.

4.0. NEW MCNPX 2.4.0 FEATURES

4.1. Summary

MCNPX 2.4.0 has several new capabilities not found in either MCNP4C or MCNPX 2.3.0 (initials of principal developers are shown in parentheses[2]). Details of these features are described in additional subsections below.

> FORTRAN 90 modularity and dynamic memory allocation (GWM);
> Distributed memory multiprocessing for the entire energy range of all particles (GWM);
> Repeated structures source path improvement (LLC/JSH);
> Default dose functions (LSW/JSH);
> Light-ion recoil (JSH);
> Enhanced color geometry plots (GWM/JSH);
> Photonuclear cross section plots (JSH);
> Proton cross section plots (JSH);

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[2] Gregg W. McKinney (GWM), John S. Hendricks (JSH), Laurie S. Waters (LSW), Leland L. Carter (LLC).

Proton reaction multipliers with FM cards (JSH);
Photonuclear reaction multipliers with FM cards (JSH/GWM);
Some speedups (GWM/JSH);
Logarithmic interpolation on input cards (JSH);
Cosine bins that may be specified in degrees (JSH);
Cosine bins may be specified for F2 flux tallies (JSH);
Source particles that may be specified by descriptors (JSH);
Pause command for tally and cross section plots (JSH); and
Correction of all known MCNPX and MCNP4C bugs/problems.

4.2. Description

4.2.1. FORTRAN 90 Modularity and Dynamic Memory Allocation

The F90 conversion provides improvements in code modularity, standardization of functions such as timing across platforms, and compiler reliability. F90 will run more slowly on some systems. Specifically, we have eliminated equivalences as a means of dynamic storage allocation by using F90 pointers and allocable arrays. We have replaced most common calls with F90 modules. The code will compile in both free and fixed F90 formats.

MCNPX 2.4.0 can be modified by patches, and as much of the MCNP4C coding as possible has been preserved so that MCNP4C patches can be applied directly to MCNPX 2.4.0.

Continuing improvements in the F90 structure are ongoing, especially where they concern physics modules that have been brought into the code.

4.2.2. Distributed Memory Multiprocessing for the Entire Energy Range of All Particles

Parallel Virtual Machine (PVM) software can be used to run the entire MCNPX code in parallel. Fault tolerance and load balancing are available, and multiprocessing can be done across a network of heterogeneous platforms. Threading may be used for problems run in the table data region only.

4.2.3. Repeated Structures Source Path Improvement

Sources in repeated structures and lattices now may be specified with the same notation as tallies, and the paths are printed correctly in the output (see Section 5.2).

4.2.4. Default Dose Functions

Fourteen standard dose functions in United States (US) or international units may be applied to any tally without entering the tables on DE/DF cards (see Section 5.1).

4.2.5. Light-Ion Recoil
Neutrons and protons undergoing elastic scatter can cause light-ion targets (H, D, T, ^{3}He, and ^{4}He) to create particles (h, d, t, s, and a) that are banked for subsequent transport with the proper two-body kinematics (see Section 5.6.2).

4.2.6. Enhanced Color Geometry Plots
Sixty-four colors are now available. Cells may be colored by any cell-based quantity, not just material. Logarithmic shading of importances, weight windows, and summary information is automatic. Color-coded shading of mesh-based weight windows is available (see Section 5.7).

4.2.7. Photonuclear Cross Section Plots
Photonuclear interaction cross sections and their secondary particle yields may now be plotted with the MCNPX cross section plotter (see Section 5.8).

4.2.8. Proton Cross Section Plots
Photonuclear interaction cross sections and their secondary particle yields may now be plotted with the MCNPX cross section plotter (see Section 5.9).

4.2.9. Photonuclear Reaction Multipliers
Photonuclear cross sections and yields may be used to multiply fluxes and other tally quantities on FM tally cards. Now the production of various secondary particles and reactions such as photofission may be tallied (see Section 5.10).

4.2.10. Proton Reaction Multipliers
Proton cross sections and yields may be used to multiply fluxes and other tally quantities on FM tally cards (see Section 5.10).

4.2.11. Speedup
The increased generality and FORTRAN 90 conversion of MCNPX 2.4.k slow the code down by ~15%. However, in certain cases, some speedups have been added to make it faster than either MCNP4C3 or MCNPX 2.3.0, particularly for repeated structures/lattice plotting and few-particle MCNPX problems.

4.2.12. Logarithmic Interpolation

        E4 1.e-5 10log 1.e5

is equivalent to

        E4 1.e-5 .0001 .001 .01 .1 1 10 100 1000 10000   .

4.2.13. Cosine Specification in Degrees
Cosine bins may be specified in degrees for F1 current tallies. Cosine bins may now also be specified for F2 flux tallies (see Section 5.4).

4.2.14. Source Particles May Be Specified by Descriptors
Previously,

      SDEF par = n,

where

      n = 1,2,...,9,...   (numbers).

Now,

      SDEF par = n,

where

      n = n,p,...,h,... (character particle designators)

is optionally allowed (see Section 5.5).

4.2.15. Pause Command for Tally and Cross Section Plots
The MCNPX geometry plot *PAUSE* command is now extended to tally and cross section plots. When the word *PAUSE N* is put in a tally plotting COM input file, the picture will display for *N* seconds. If the command *PAUSE* (without the *N*) is in the COM file, then the display will hold until a key is struck.

5.0.   USER INTERFACE FOR NEW MCNPX 2.4.0 FEATURES

Section 4 provided a summary description of the new MCNPX 2.4.0 features. This section now describes the user interface changes for the following subset of those features.

      default dose functions: DFn;
      repeated structures source specification: SDEF, SI;
      logarithmic interpolation: Nlog;
      expanded cosine specification: Cn;
      SDEF particle specification: SDEF par h;
      energy straggling: PHYS:N 4j I;
      light ion recoil: PHYS: N 6j R;
      enhanced color geometry plots: COLOR;
      photonuclear cross section plots;
      proton cross section plots; and
      photonuclear and proton reaction multipliers: FM.

These features are described below and in the forthcoming new MCNPX 2.4.0 manual.

5.1. Default Dose Functions

The MCNPX DFACT mesh tally capability has been expanded to provide standard dose conversions with the DE/DF cards.

Users may input a table as in MCNP/MCNPX (although the interpolation int = log or int = lin may now be placed anywhere). n = tally number, which implies particle type.

> DEn E1 E2 int E3 ...
> DFn F1 int F2 F3 ...

Or, the following DF card is accepted:

> DFn iu=j fac=F int ic=I   ,

where the following entries are all optional.

> iu = 1 = US units (rem/h)
> iu = 2 = international units (sieverts/h)
> Default: iu = 2 international units (sieverts/h)

> fac = normalization factor for dose (acr is also accepted instead of fac).
> fac = -1 = normalize results to Q = 20 by dividing the parametric form of Q
> $[5.0+17.0*exp(-(ln(2E))*2/6)]$ from ICRP60 (1990), paragraph A12.
> fac = -2 = apply LANSCE albatross response function.
> Default: fac = 1.0.

> int = "log" or "lin" results in "log" or "lin" interpolation of energy; the dose
>   function is always linear. That is, "lin" results in "linlin" interpolation, and
>   "log" results in "loglin" interpolation.

> Default: for ic = 10, 40: log
> for ic = 20,31-39: recommended analytic parameterization.

ic = i = standard dose function.

> <u>i neutron dose function</u>
> 10 = ICRP-21 1971
> 20 = NCRP-38 1971, ANSI/ANS-6.1.1-1977
> 31 = ANSI/ANS-6.1.1-1991 (AP anterior-posterior)
> 32 = (PA posterior-anterior)
> 33 = (LAT side exposure)
> 34 = (ROT normal to length and rotationally symmetric)

40 = ICRP-74 1996 ambient dose equivalent

<u>i photon dose function</u>
10 = ICRP-21 1971
20 = Claiborne & Trubey, ANSI/ANS 6.1.1-1977
31 = ANSI/ANS-6.1.1-1991 [AP (anterior-posterior)]
32 = PA (posterior-anterior)
33 = (LAT side exposure)
34 = (ROT normal to length and rotationally symmetric)
35 = (ISO isotropic)

Default: ic = 10

5.1.1. Examples

DF4

DF0 ic 40 iu 1 lin fac 123.4

DF1 iu=2 acr=-2 log ic=34

5.2.   Repeated Structures Source Specifications

The CEL source specification for repeated structures geometries is now consistent with the tally specification. The old MCNP4C specification still works, but the new one is

```
sdef  cel=d3  pos=0 6 0 ext d1 rad d2 axs 0 1 0
si3 L (1<10[0 0 0]<11) (1<10[1 0 0]<11) (1<10[2 0 0]<11)
(1<10[0 1 0]<11) (1<10[1 1 0]<11) (1<10[2 1 0]<11)
```

All of the output prints now also are consistent.

5.3.   Logarithmic Interpolation

Logarithmic interpolation is now allowed on input cards. It is similar to the IJMR interpolation of MCNP. For example,

```
e0    1.e-3 6log 1.e4
```

is interpreted as

```
e0  .001 .01 .1 1 10 100 1000 10000  .
```

5.4. Expanded Cosine Specification

Cosines may now be specified in degrees. They may also now be specified with flux tallies:

  *C2 150 120 90 60 30 0   .

The * on the C2 card interprets cosines as in degrees. Entries must be such that the cosine is monotonically increasing.

5.5. SDEF Particle Specification

The source particle type now may be specified on the SDEF card by its symbol:

  SDEF par=h

5.6. PHYS:n Changes

For neutrons, the fifth entry is the model/table energy cutoff (see new Print Table 41). In previous MCNPX versions, this was the third PHYS:N entry.

For particle types n > 2 (e,…, h,…), the fifth entry is the energy straggling (see Section 5.6.1).

For neutrons or protons, the seventh entry is the light-ion recoil control (see Section 5.6.2).

5.6.1. Energy Straggling (Particle Types n > 2)
Dick Prael's and Grady Hughes's energy-straggling model in MCNPX 2.2.6 and later is specified as follows.

  PHYS:n 4j I   (5th entry on PHYS:n card) ,

where

>   I = 0: Prael's new straggling model—an energy correction addressing stopping powers of charged particles (default)

>   = 1: continuous slowing down ionization model; and

>   = -1: straggling model used in MCNPX 2.2.4 and previous releases.

n = particle type:

for

n = N, entry I is the library energy cutoff (formerly the third entry);

n = P, entry I is unused; and

n = E, the straggling model control is the same as MCNPX 2.3.0 and MCNP4C3.

5.6.2. Light-Ion Recoil (Incident Neutrons and Protons only)

PHYS:n 6j R   (seventh entry on PHYS:n card)   ,

where

n = N or H (neutrons and protons only);

0 < R ≤ 1: number of light-ion particles (h, d, t, s, and a) to be created at each elastic scatter on light nuclei for H, D, T, ^{3}He, and ^{4}He. The ionization potential is accounted for, and the proper two-body kinematics is used (with neutron free-gas thermal treatment if appropriate) to bank the created particles with the proper energy and angle.

Auxiliary cards:

  mode n h d t s a ,

    where n and/or h is required to produce light-ion elastic recoil from either neutrons and/or protons, and

    h,d,t,s,a are required to produce any of these particles.

Note that protons colliding with hydrogen to produce more protons can produce an overwhelming number of protons; caution is required.

  cut:N 2j 0   ,

where

    N = h,d,t,s,a may be needed to produce low-energy elastic recoil ions. The default alpha (a) energy cutoff is 4 MeV; however, dropping the alpha cutoff to

zero will result in the minimum energy cutoff for an alpha of 1 keV, thus enabling the creation of E > 1 keV alphas.

5.7.   Enhanced Color Geometry Plots (D-10:JSH-2002-09)

The new plotting capabilities are accessible via either the interactive geometry plot capability or the command/prompt interface.

In the interactive capability, the "SCALES n" button has been moved up two lines (after the cursor) to make room for a larger "COLOR name" button. The default is "COLOR mat", which colors problem cells by the program material number. This button must be clicked to get "COLOR off" (black and white) and then clicked again to color by whatever parameter is listed after the "Edit" button. For example, in the right margin, "cel" must be clicked, which will make the "Edit" quantity "cel". Next, "COLOR" must be clicked so that it says "COLOR cel"; on the next plot, the color shades will be by program cell number.

In the command/prompt input mode, the label command must be set, such as

PLOT> label 0 1 rho;

then the color command must be set such as

PLOT> color on

and the coloring will now be by rho, the atom density.

5.8.   Photonuclear Cross Section Plots (D-10:JSH-02-98)

Until now the only photon cross sections that could be plotted in MCNPX. Photoatomic reaction numbers are all negative: -1 = incoherent, -2 = coherent, -3 = photoelectric, -4 = pair production, -5 = total, -6 = heating. For the MCNPX photonuclear cross section plotting, the reaction numbers are all positive. The principal photonuclear cross sections are: 1 = total, 2 = nonelastic, 3 = elastic, 4 = heating, >4 = various reactions such as 18 = (γ,f).   The photonuclear yields (multiplicities) for various secondary particles are specified by adding 1000 x the secondary particle number to the reaction number. For example, 31001 is the total yield of deuterons (particle type d = 31); 34001 is the total yield of alphas (particle type α = 34); 1018 is the total number of neutrons (particle type n = 1) from fission. To find out which reactions are available for a particular nuclide or material, enter an invalid reaction number, such as mt = 99, and MCNPX will list the available photonuclear reactions and the available yields such as 1018, 31018, 34018. Entering a bad nuclide, xs = 12345.67u, will cause MCNPX to list the available nuclides.

The figures below illustrate photonuclear cross section plots for mt = 1 and mt = 2005.

.

cross section plot

photonuclear total cross section

cross section plot

photonuclear reaction cross section
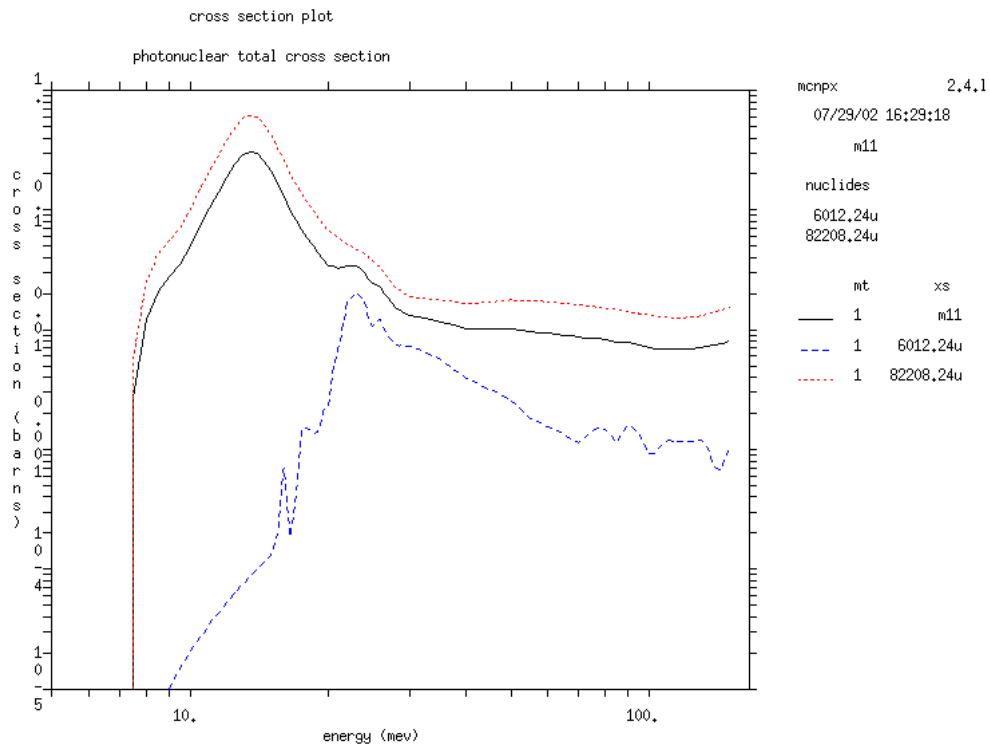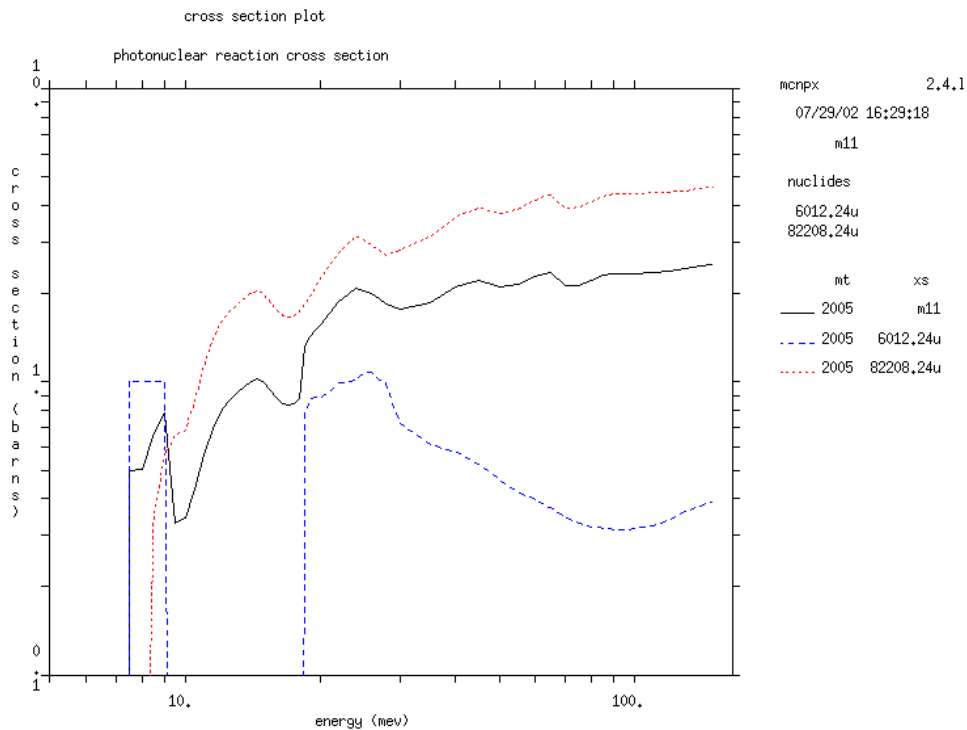
5.9. Proton Cross Section Plots (D-10:JSH-02-98)

For proton cross section plotting, the reaction numbers are similar to the neutron reaction numbers: all positive. The principal photonuclear cross sections are: ± 1 = total, ± 2 = nonelastic, ± 3 = elastic, ± 4 = heating, >4 = various reactions. On the LA150H proton library, the only available reaction is mt = 5 and its multiplicities, 1005, 9005, 31005, etc. The multiplicity reaction numbers for interaction reaction mt = 5 are 1005 for neutrons, n = 1, 9005 for protons, h = 9, 31005 for deuterons, d = 31, etc. To find out which reactions are available for a particular nuclide or material, enter an invalid reaction number, such as mt = 99, and MCNPX will list the available proton reactions and the available yields such as 1005, 32001, 34002, etc. The proton multiplicity, mt = 9001, 9004, 9005, etc., is generally available along with the total cross section and heating number, mt = 1, mt = 4. Entering a bad nuclide, xs = 12345.67h, will cause MCNPX to list the available proton nuclides.

5.10. Photonuclear and Proton Reaction Multipliers (D-10:JSH-02-98)

Photonuclear and proton cross sections may be used in tally multipliers on the FM card. For example,

    M102 92235 1 pnlib=27u
    F2:P 1

FM2   (-1 102 18 1018)

 It is always wise to plot the desired cross sections first to see if they are available with the expected reaction numbers in the data library. The tally multipliers treat the data the same way as the data are treated in transport: the cross section at the lowest energy is extended down to E = 0 for protons with mt < 0; the cross section at the highest energy of the table is extended to E = ∞ for proton interaction cross sections with mt < 0 and for photonuclear interaction cross sections, mt < 1000. These extrapolations can be seen in the cross section plots.

6.0.   FUTURE WORK

- **Mix-and-match capability:** In the neutron (and other particle) energy range above the top energy of some data libraries but below the top energy of other libraries, MCNPX currently cannot mix both model and tabular data. Either the higher-energy data are ignored and models are used for all nuclides or the data are used where they exist and are extrapolated from the top of the energy table for nuclides where the data do not exist. A means of mixing and matching both tabular data and model data is being developed.

- CEM 2K: The current CEM physics model is being updated.
- Pulse height tallies with variance reduction.
- Cugnon Intranuclear Cascade (INC) model and Schmidt evaporation model.
- Special features for Space applications.
- A capability to continue runs that write HTAPE files
- Integration of HTAPE tallies directly into MCNPX.
- Heavy ion tracking and interactions.
- Improved high energy physics with the LAQGSM model.

7.0.   ACKNOWLEDGEMENTS

LANL nuclear data and physics teams (Mark Chadwick, Robert C. Little, Stepan Mashnik, David Madland, Arnie Sierk, Morgan White). John Hendricks and Gregg McKinney (now actively working on MCNPX) were the principal developers and leaders of MCNP for the past decade.

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